# Non-equilibrium dynamics of the Bose-Hubbard model: A projection operator approach


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We study the phase diagram and non-equilibrium dynamics, both subsequent to a sudden quench of the hopping amplitude $J$ and during a ramp $J(t) = Jt/\tau$ with ramp time $\tau$, of the Bose-Hubbard model at zero temperature using a projection operator formalism which allows us to incorporate the effects of quantum fluctuations beyond mean-field approximations in the strong coupling regime. Our formalism yields a phase diagram which provides a near exact match with quantum Monte Carlo results in three dimensions. We also compute the residual energy $Q$, the superfluid order parameter $\Delta(t)$, the equal-time order parameter correlation function $C(t)$, and the wavefunction overlap $F$ which yields the defect formation probability $P$ during non-equilibrium dynamics of the model. We find that $Q$, $F$, and $P$ do not exhibit the expected universal scaling. We explain this absence of universality and show that our results compare well with recent experiments.



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Ultracold atoms in optical lattices provide us with an unique setup to study non-equilibrium quantum dynamics of closed quantum systems [1, 2]. The theoretical study of such quantum dynamics has seen great progress in recent years [3]. Most of these theoretical works have either restricted themselves to the physics of integrable and/or one-dimensional (1D) models or concentrated on generic scaling behavior of physical observables for sudden or slow dynamics through a quantum critical point (QCP) [3]. However, quantum dynamics of specific experimentally realizable non-integrable models in higher spatial dimension $d$ and strong coupling regime have not been studied extensively. The Bose-Hubbard model with on-site interaction strength $U$ and nearest neighbor hopping amplitude $J$, which provides an accurate description for ultracold bosons in an optical lattice, constitutes an example of such models [4]. Most of the studies on dynamics of this model have concentrated on numerics for $d \leq 2$ [5, 6], weak coupling regime [7], and mean-field description of quench dynamics in the strong coupling regime [8, 9]. Recent experiments [2] on higher dimensional Bose-Hubbard models in the strong-coupling regime ($U \gg J$) clearly necessitate computation of dynamical evolution of several quantities beyond the mean-field theory and for arbitrary ramp time $\tau$. To the best of our knowledge, such a study has not been carried out.

In this work we present a theoretical formalism beyond mean-field theory, which enables us to investigate in a semi-analytic way, at equal footing, both the equilibrium phase diagram and the non-equilibrium dynamics of the Bose-Hubbard model in the strong coupling regime and at zero temperature. The central results of our work are the following. First, we compute the equilibrium phase diagram and demonstrate that it provides a near perfect match to the corresponding quantum Monte Carlo (QMC) results [10] in three dimensions (3D). Second, we apply our formalism to non-equilibrium dynamics of the model for a finite ramp $J(t) = Jt/\tau$ from $t = t_i$ to $t = t_f$. We compute the residual energy $Q$ and the wavefunction overlap $F$ [*i.e.* the overlap between the system wavefunction after the ramp and the corresponding ground state wavefunction with $J = J(t_f)$] which also yields the defect formation probability $P = 1 - F$ [3] as functions of $\tau$. We show that for slow ramps $P$ reaches a plateau, showing absence of expected scaling behavior [3]. We qualitatively explain such an absence of universal scaling and relate it to the recent experimental observations of Ref. [2]. Finally, we show that our formalism allows us to address the time evolution of the bosons after a sudden quench from the Mott ($J = J_i$) to the superfluid ($J = J_f$) phase through the tip of the Mott lobe. We compute the order parameter $\Delta(t)$ and the equal-time order parameter correlation function $C(t)$ during such an evolution. We also compute $F$ and $Q$ for a sudden quench from the critical point ($J_i = J_c$) to the superfluid phase and show that they agree to the finite ramp results in the limit of small $\tau$ and do not exhibit universal scaling behavior [11]. We note that dynamical properties of the Bose-Hubbard model for $d > 2$ in the strongly coupled regime have not been addressed beyond mean-field theory so far; our semi-analytical results therefore constitute significant extension of our understanding of the dynamics of this model in the strong-coupling regime.

The Hamiltonian of the Bose-Hubbard model is

$$\mathcal{H} = \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} -J b^\dagger_{\mathbf{r}} b_{\mathbf{r}'} + \sum_{\mathbf{r}} [-\mu \hat{n}_{\mathbf{r}} + \frac{U}{2} \hat{n}_{\mathbf{r}} (\hat{n}_{\mathbf{r}} - 1)], \quad (1)$$

where $b$ ($\hat{n}$) is the boson annihilation (number) operator living on the sites of a $d$-dimensional hypercubic lattice, and the chemical potential $\mu$ fixes the total number of particles. The corresponding many-body Schrödinger equation $i\hbar\partial_t|\psi\rangle = \mathcal{H}|\psi\rangle$ is difficult to handle even numerically due to the infinite dimensionality of the Hilbert space. A typical practice is to use the Gutzwiller ansatz

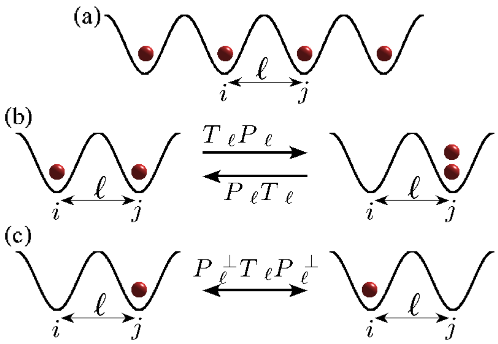


FIG. 1: (Color online) (a) Schematic representation of the Mott state with $\bar{n} = 1$. (b) Typical hopping process mediated via $T_\ell^0$. (c) Hopping process mediated via $P_\ell^\perp T_\ell P_\ell^\perp$. Notice that the states in (c) become part of the low-energy manifold near the critical point, while those in the right side of (b) do not and are always at an energy $U$ above the Mott state.

$|\psi\rangle = \prod_{\mathbf{r}} \sum_n c_n^{(\mathbf{r})} |n\rangle$ and solve for $c_n^{(\mathbf{r})}$ keeping a finite number of states $n$ around the Mott occupation number $n = \bar{n}$. This yields the standard mean-field results with $c_n^{(\mathbf{r})} = c_n$ for homogeneous phases of the model [12].

To build in fluctuations over such a mean-field theory, we use a projection operator technique [13]. The key idea behind this approach is to introduce a projection operator $P_\ell = |\bar{n}\rangle\langle\bar{n}|_{\mathbf{r}} \times |\bar{n}\rangle\langle\bar{n}|_{\mathbf{r}'}$, which lives on the link $\ell$ between the two neighboring sites $\mathbf{r}$ and $\mathbf{r}'$. The effect of $P_\ell$ is to project any state of the system to the manifold of states for which $n_{\mathbf{r}}, n_{\mathbf{r}'} = \bar{n}$. Using $P_\ell$, one can rewrite the hopping term of $\mathcal{H}$: $T' = \sum_{\langle \mathbf{r}\mathbf{r}'\rangle} -J b_{\mathbf{r}}^\dagger b_{\mathbf{r}'} = \sum_\ell T_\ell = \sum_\ell [(P_\ell T_\ell + T_\ell P_\ell) + P_\ell^\perp T_\ell P_\ell^\perp]$, where $P_\ell^\perp = (1 - P_\ell)$. Note that, as schematically explained in Fig. 1, in the strong-coupling regime, the term $T_\ell^0[J] = (P_\ell T_\ell + T_\ell P_\ell)$ represents hopping processes which take the system out of the low-energy manifold [13]. To obtain an effective low energy Hamiltonian, we therefore devise a canonical transformation via an operator $S \equiv S[J] = \sum_\ell i[P_\ell, T_\ell]/U$, which eliminates $T_\ell^0[J]$ to first order in $z_0 J/U$, where $z_0 = 2d$ is the coordination number of the lattice. This leads to the effective Hamiltonian $H^* = \exp(iS)\mathcal{H}\exp(-iS)$ up to $\mathrm{O}(z_0^2 J^2/U)$

$$\begin{aligned} H^* &= H_0 + \sum_\ell P_\ell^\perp T_\ell P_\ell^\perp - \frac{1}{U}\sum_\ell \Big[ P_\ell T_\ell^2 + T_\ell^2 P_\ell \\ &- P_\ell T_\ell^2 P_\ell - T_\ell P_\ell T_\ell \Big] - \frac{1}{U}\sum_{\langle \ell\ell'\rangle} \Big[ P_\ell T_\ell T_{\ell'} - T_\ell P_\ell T_{\ell'} \\ &+ \frac{1}{2}\Big( T_\ell P_\ell P_{\ell'} T_{\ell'} - P_\ell T_\ell T_{\ell'} P_{\ell'} \Big) + \mathrm{h.c.} \Big], \end{aligned} \qquad (2)$$

where $H_0$ denotes the on-site terms in Eq. 1. Using $H^*$ one can now compute the ground state energy $E = \langle\psi|\mathcal{H}|\psi\rangle = \langle\psi'|H^*|\psi'\rangle + \mathrm{O}(z_0^3 J^3/U^2)$, where

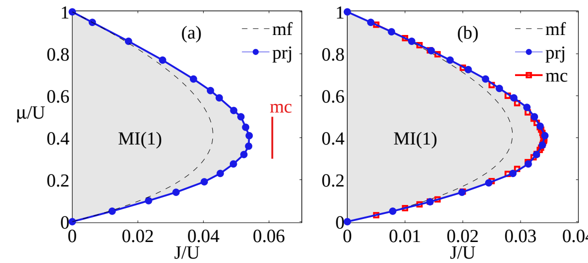


FIG. 2: (Color online) Phase diagram of the Bose-Hubbard model in 2D (a) and 3D (b). The blue dots and blue solid lines (black dashed line) indicate the phase diagram obtained by the projection operator (mean-field) method. The red squares indicate QMC data.

$|\psi'\rangle = \exp(iS)|\psi\rangle$. We use a Gutzwiller ansatz

$$|\psi'\rangle = \prod_{\mathbf{r}} \sum_n f_n^{(\mathbf{r})} |n\rangle, \qquad (3)$$

so that $|\psi'\rangle = |\psi\rangle$ only in the Mott limit ($S, J = 0$) and the energy becomes a functional of the coefficients

$$E[\{f_n\}; J] = \langle\psi'|H^*|\psi'\rangle. \qquad (4)$$

The contributions to $E[\{f_n\}; J]$ from the first two terms in $H^*$ (Eq. 2) represent the mean-field energy functional, while the rest of the terms yield contributions due to quantum fluctuations. Thus the method constitutes systematic inclusion of effects of quantum fluctuation over mean-field theory. The phase diagram obtained by minimizing $E[\{f_n\}; J]$ with respect to $\{f_n\}$ for 2D(3D) and $\bar{n} = 1$ is shown in Fig. 2(a)(Fig. 2(b)). We find that the match with QMC data [10] is nearly perfect in 3D (with an error of $\sim 0.05\%$ at the tip of the Mott lobe) where mean-field theory provides an accurate starting point. In contrast, for 2D, we find $J_c/U = 0.055$ compared to the QMC value 0.061 (red line in Fig. 2(a)). Here the match with QMC is not as accurate; however it compares favorably to other analytical methods [15]. For the rest of this work, we shall restrict ourselves to $d = 3$ and $\bar{n} = 1$.

Next, we apply our formalism to address the dynamics of the model during a ramp with finite rate $\tau^{-1}$. We consider a ramp process under which $J$ evolves from $J_i$ at $t_i = 0$ to $J_f$ at $t_f = \tau$:$J(t) = J_i + (J_f - J_i)t/\tau$. To solve the Schrödinger equation, we make a time-dependent canonical transformation via a time-dependent $S[J(t)]$ to eliminate $T_\ell^0$ up to first order from $\mathcal{H}$ *at each instant*. This yields the Schrödinger equation

$$(i\hbar\partial_t + \partial S/\partial t)|\psi'\rangle = H^*[J(t)]|\psi'\rangle. \qquad (5)$$

The additional term $\partial S/\partial t$ takes into account the possibility of creation of excitations during the time evolution with a finite ramp rate $\tau^{-1}$. The above equation yields an accurate description of the ramp with $H^*[J(t)]$ given by Eq. 2 for $J(t)/U \ll 1$. Note that this does not impose a constraint on $\tau$; it only restricts $J_f/U$ and $J_i/U$, to

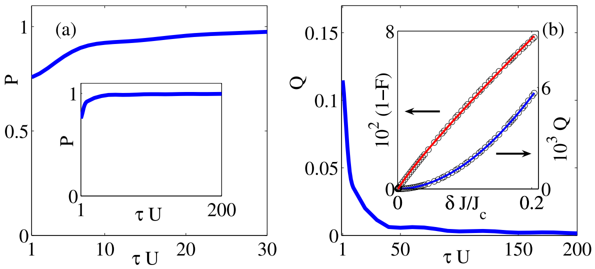


FIG. 3: (Color online) (a) Plot of $P$ as a function $\tau U$ (in units of $\hbar = 1$) for $J_i/U = 0.05$ (SF phase) and $J_f/U = 0.005$ (Mott phase) showing the plateau-like behavior at large $\tau$, and the corresponding saturation of $Q$ (b). The inset in (b) shows $Q$ and $1 - F$ as a function of $\delta J/J_c$ for $\tau U = 1$.

be small. Thus the method can treat both "slow" and "fast" ramps at equal footing.

Substituting Eq. 3 into Eq. 5 and allowing for time-dependent $f_n^{(\mathbf{r})}$, we find that the evolution of the system is given by the set of coupled equations

$$\begin{aligned} i\hbar\partial_t f_n^{(\mathbf{r})} &= \delta E[\{f_n(t)\}; J(t)]/\delta f_n^{*(\mathbf{r})} + \frac{i\hbar}{U}\frac{\partial J(t)}{\partial t} \\ &\times \sum_{\langle \mathbf{r}'\rangle_{\mathbf{r}}} \sqrt{n} f_{n-1}^{(\mathbf{r})}\Big[\delta_{n\bar{n}}\varphi_{\mathbf{r}'\bar{n}} - \delta_{n,\bar{n}+1}\varphi_{\mathbf{r}',\bar{n}-1}\Big] \\ &\quad + \sqrt{n+1} f_{n+1}^{(\mathbf{r})}\Big[\delta_{n\bar{n}}\varphi^*_{\mathbf{r}',\bar{n}-1} - \delta_{n,\bar{n}-1}\varphi^*_{\mathbf{r}'\bar{n}}\Big], \end{aligned} \tag{6}$$

where $\varphi_{\mathbf{r}} = \langle\psi'|b_{\mathbf{r}}|\psi'\rangle = \sum_n \varphi_{\mathbf{r}n} = \sum_n \sqrt{n+1} f_{\mathrm{n}}^{*(\mathbf{r})} f_{\mathrm{n+1}}^{(\mathbf{r})}$, and $\delta_{nn'}$ is the Kronecker delta.

Using Eq. 6, we solve for $f_n^{(\mathbf{r})} \equiv f_n$ for translationally invariant systems numerically keeping all states $0 \le n \le 5$ with $\bar{n} = 1$. Using these, we compute the defect formation probability $P = 1 - F = 1 - |\langle\psi_G|\psi(t_f)\rangle|^2$, where $|\psi_G\rangle$ ($|\psi(t_f)\rangle$) denotes the final ground state (state after the ramp), for a ramp from $J_i/U = 0.05$ (superfluid phase) to $J_f/U = 0.005$ (Mott phase) as a function of $\tau$. We find that $P$ exhibits a plateau like behavior at large $\tau$ and do not display universal scaling as expected from generic theories of slow dynamics of quantum systems near critical point [3]. This seems to be in qualitative agreement with the recent experiments presented in Ref. [2], where ramp dynamics of ultracold bosons from superfluid to the Mott region has been experimentally studied. Indeed, it was found, via direct measurement of $\bar{n}$ per site, that $P$ displays a plateau like behavior similar to Fig. 3(a) [the inset displays the saturation for longer $\tau$]. In Fig. 3(b), we show the analogous saturation and lack of universal scaling of the residual energy $Q = \langle\psi_f|\mathcal{H}[J_f]|\psi_f\rangle - E_G[J_f]$, where $E_G[J_f]$ denotes the ground state energy at $J = J_f$ as obtained by minimizing $E[\{f_n\}; J_f]$ in Eq. 4.

Such a lack of universality in the dynamics can be qualitatively understood from the absence of contribution of the critical ($\mathbf{k} = 0$) modes. In the strong-coupling regime ($J/U \ll 1$), the system can access the $\mathbf{k} = 0$ modes after a time $\mathcal{T}$, which can be roughly estimated as the time

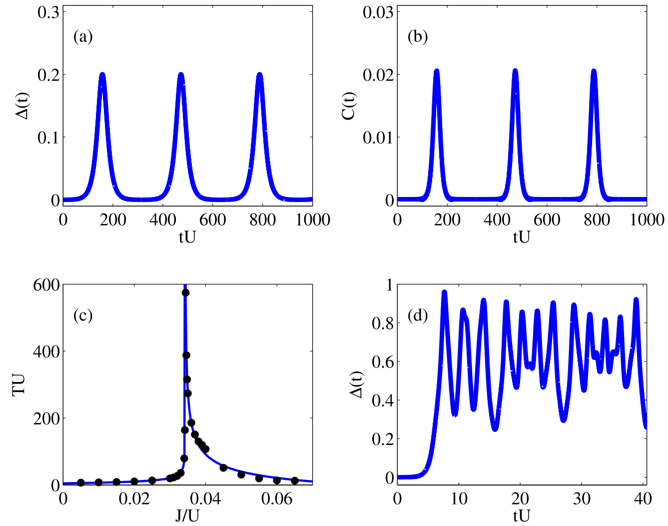


FIG. 4: (Color online) Plot of $\Delta(t)$ (a) and $C(t)$ (b) as a function of $tU$, for $J_f = 1.02J_c$. (c) The time period $T$ of the oscillations of $\Delta(t)$. (d) Same as in (a) for $J_f = 3.51J_c$. We have set $\hbar = 1$ for all plots.

taken by a boson to cover the linear system dimension $L$. For typical small $J$ ($U = 1$) in the Mott phase and near the QCP, $\mathcal{T} \sim \mathrm{O}(L\hbar/J)$ can be very large. Thus for $t \le \mathcal{T}$, the dynamics, governed by local physics, which is well captured by our method, do not display critical scaling behavior. We note that in realistic experimental setups in the deep Mott limit [2], $\mathcal{T}$ may easily exceed the system lifetime making observation of universal scaling behavior impossible in such setups.

We now apply this method to address the dynamics of the model after a sudden quench [14], from $J_i$ (Mott phase) to $J_f$ (superfluid phase) through the tip of the Mott lobe, where the dynamical critical exponent $z = 1$. The time evolution of the order parameter $\Delta_{\mathbf{r}}(t) = \langle\psi(t)|b_{\mathbf{r}}|\psi(t)\rangle = \langle\psi'(t)|b'_{\mathbf{r}}|\psi'(t)\rangle$, where $b'_{\mathbf{r}} = \exp(iS[J_f])b_{\mathbf{r}}\exp(-iS[J_f])$, can then be expressed in terms of $f_n^{(\mathbf{r})}$ as

$$\begin{aligned} \Delta_{\mathbf{r}}(t) &= \varphi_{\mathbf{r}}(t) + J/U \sum_{\langle \mathbf{r}'\rangle_{\mathbf{r}}} \bar{n}\Big[|f_{\bar{n}}^{(\mathbf{r})}|^2 - f_{\bar{n}-1}^{(\mathbf{r})}|^2\Big]\varphi_{\mathbf{r}'\bar{n}} \\ &+ (\bar{n}+1)\Big[|f_{\bar{n}}^{(\mathbf{r})}|^2 - f_{\bar{n}+1}^{(\mathbf{r})}|^2\Big]\varphi_{\mathbf{r}',\bar{n}-1} + \Big[\Phi_{\mathbf{r},\bar{n}-2} \\ &- \Phi_{\mathbf{r},\bar{n}-1}\Big]\varphi^*_{\mathbf{r}'\bar{n}} + \Big[\Phi_{\mathbf{r}\bar{n}} - \Phi_{\mathbf{r},\bar{n}-1}\Big]\varphi^*_{\mathbf{r}',\bar{n}-1}, \end{aligned} \tag{7}$$

where $\Phi_{\mathbf{r}n} = \sqrt{(n+1)(n+2)} f_{\mathrm{n}}^{*(\mathbf{r})} f_{\mathrm{n+2}}^{(\mathbf{r})}$. Note that the first term in Eq. 7 represents the mean-field result. The role of quantum fluctuations in the evolution of $\Delta_{\mathbf{r}}(t)$ becomes evident in computing the equal-time order parameter correlation function $C_{\mathbf{r}}(t) = \langle\psi'(t)|b'_{\mathbf{r}}b'_{\mathbf{r}}|\psi'(t)\rangle - \Delta^2_{\mathbf{r}}(t)$. To compute $\Delta_{\mathbf{r}}(t)$ and $C_{\mathbf{r}}(t)$, we solve Eq. 6 numerically for a translationally invariant system. The resultant plot of $\Delta_{\mathbf{r}}(t) \equiv \Delta(t)$ is shown in Fig. 4(a)[(d)] for $J_i = 0$ and $J_f/J_c = 1.02 (J_f/J_c = 3.51)$. We find

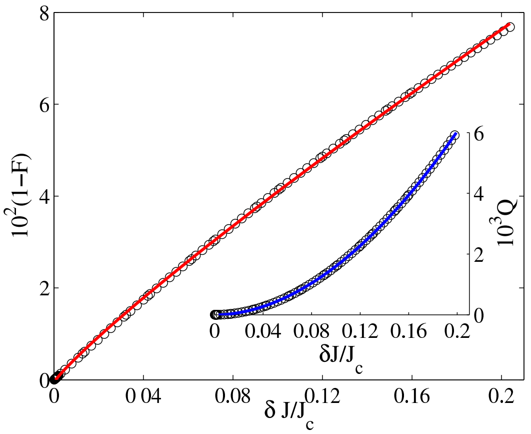


FIG. 5: (Color online) Plot of $1-F$ and $Q$ as a function of the $\delta J$ for $\delta J/J_c \ll 1$. The lines correspond to fits yielding a power $1-F(Q) \sim (\delta J)^{r_1(r_2)}$ with $r_1 \simeq 0.89$ and $r_2 \simeq 1.9$.

that near the critical point, $\Delta(t)$ displays oscillations with a single characteristic frequency [8], while away from the critical point ($J_f/J_c = 3.51$), multiple frequencies are involved in its dynamics. The time period $T$ (Fig. 4(c)) of these oscillations near $J_c$ is found, as a consequence of critical slowing down, to have a divergence $T \sim |J_f - J_i|^{-z\nu} = \delta J^{-0.35\pm0.05}$, leading to $z\nu = 0.35 \pm 0.05$ for $d = 3$ [3]. Finally, in Fig. 4(b) we plot $C_{\mathbf{r}}(t) \equiv C(t)$ as a function of $t$, for $J_f = 1.02J_c$. We find that $|C(t)/\Delta^2(t)|$ may be as large as 0.5 at the tip of the peaks of $\Delta(t)$, which shows strong quantum fluctuations near the QCP.

Next, we compute the wavefunction overlap $F = |\langle\psi_f|\psi_c\rangle|^2 = |\langle\psi'_f|e^{iS[J_f]}e^{-iS[J_c]}|\psi'_c\rangle|^2$ for a sudden quench starting at the QCP. Here $|\psi_f\rangle(|\psi_c\rangle)$ denotes the ground state wavefunction for $J = J_f(J_c)$. We also compute the residual energy $Q = \langle\psi_c|\mathcal{H}[J_f]|\psi_c\rangle - E_G[J_f]$, and in Fig. 5 we plot $1-F$ and $Q$ for the homogeneous case as a function of $\delta J = |J_f - J_c|$, for $\delta J/J_c \lesssim 0.2$. A numerical fit of these curves yields $1-F \sim \delta J^{0.89}$, and $Q \sim \delta J^{1.90}$, which disagrees with the universal scaling exponents ($1-F \sim \delta J^{d\nu}$ and $Q \sim \delta J^{(d+z)\nu}$) expected from sudden dynamics across a QCP with $z = 1$ [11]. Note that our results for the sudden quench match with those for the ramp dynamics at small $\tau$, shown in the inset of Fig. 3(b). In particular, the exponents obtained from the two cases are nearly identical, reflecting accurate reproduction of fast ramp dynamics in the sudden quench limit.

Finally, we estimate the range of physical temperatures for which the zero temperature theory is accurate. For typical lattice depths in the Mott or critical regimes, $U \sim 2$ kHz $\simeq 200$nK [1]. This yields, in 3D, a melting temperature $T^* \simeq 0.2U = 40$nK for the Mott phase and a critical temperature $T_c \simeq z_0 J_c \simeq 35$nK for the SF phase at the Mott tip [16]. This requires the system temperature to be a few nano-Kelvins (and $\ll T^*$, $T_c$) , which is well within the current experimental limit $\sim 1$nK [16].

In conclusion, we have presented a projection operator formalism that describes in a semi-analytical way both the phase diagram, and non-equilibrium dynamics of the Bose-Hubbard model. It produces a phase diagram which is nearly identical to the QMC results in 3D, and allows computation of several quantities such as $F$, $Q$, $\Delta(t)$, $P$, and $C(t)$ for non-equilibrium dynamics. Its prediction for $P$ for a slow ramp matches qualitatively with recent experiments. The method, in principle, can be generalized to correlated systems which allow perturbative treatment of fluctuations and for studying ultracold bosons in a finite trap. We leave such considerations for future study.

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